

Inner product quadratures

Yu Chen

Courant Institute of Mathematical Sciences
New York University

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Abstract

We introduce a n -term quadrature to integrate inner products of n functions, as opposed to a Gaussian quadrature to integrate $2n$ functions. We will characterize and provide computational tools to construct the inner product quadrature, and establish its connection to the Gaussian quadrature.

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1 The inner product quadrature

We consider three types of n -term Gaussian quadratures in this paper,

- Type-1: to integrate $2n$ functions in interval $[a, b]$.
- Type-2: to integrate n^2 inner products of n functions.
- Type-3: to integrate n functions against n weights.

For these quadratures, the weight functions u are not required positive definite. Type-1 is the classical Guassian quadrature, Type-2 is the inner product quadrature, and Type-3 finds applications in imaging and sensing, and discretization of integral equations.

In this section we will introduce and characterize the Type-2, inner product quadrature. §2 presents algorithms for constructing the quadrature. §3 establishes framework to link the first two types, and introduce the Type-3 quadrature. §4 illustrates our quadrature design method with several examples. §5 explores generalizations of our quadrature methods to higher dimensions and examines applications to inverse scattering problems.

1.1 Notation

For $x \in [a, b]$ and $k \in [\alpha, \beta]$, by the usual abuse of notation we will denote by $G(k, x)$ the four related objects

1. A family of L^2 functions on $[a, b]$, with $k \in [\alpha, \beta]$
2. The linear subspace spanned by these functions;
3. The kernel of an integral operator;
4. The matrix of that operator of size $[\alpha, \beta]$ -by- $[a, b]$.

When k in $G(k, x)$ takes on some finite n values k_j in $[\alpha, \beta]$, the resulting set of n functions are denoted by

$$T(n, x) = \{ G(k, x), x \in [0, 1], k = k_j, j = 1 : n \} \quad (1)$$

Viewed as a matrix of size n -by- $[a, b]$, $T(n, x)$ has infinite number of columns, and its n rows consist of the n functions $T_j(x)$ in $L^2[a, b]$. For example, when k ranges from 0 to $n - 1$, the power functions

$$G(k, x) = \{ x^k, \quad x \in [0, 1], \quad k \in [\alpha, \beta] \} \quad (2)$$

becomes $T(n, x) = \Pi_n$, polynomials of degree less than n . Similarly, when k takes on integers, the pure tones

$$G(k, x) = \{ \exp(ikx), \quad x \in [-\pi, \pi], \quad k \in [-\beta, \beta] \} \quad (3)$$

becomes trigonometric polynomials. We will first consider a n -term quadrature to integrate the inner products in $T(n, x)$.

For $c \in [a, b]$, the column of $T(n, x)$ taken at $x = c$ is the n -by-1 vector

$$T(n, c) = T(n, x)|_{x=c} \quad (4)$$

Given a weight function u we define the dot product in $T(n, x)$

$$f \cdot g = \int_a^b u(x) f(x) \bar{g}(x) dx \quad (5)$$

When u is positive, (5) will be adopted as the inner product for $L^2[a, b]$.

Given n distinct points x_j , $j = 1 : n$ in $[a, b]$, let $T(n, \{x_j\})$ be the n -by- n matrix formed by the n columns $T(n, x_j)$, $j = 1 : n$.

Let $B(n, n)$ be the n -by- n Gramian matrix of the n functions $T_j(x)$ so that

$$B(n, n) = T(n, x) \cdot T(x, n) \quad (6)$$

where $T(x, n)$ is the complex transpose of $T(n, x)$. Note that the dot sign requires inner product (5) with the underlying weight function u . For real valued u , B is Hermitian.

For positive u , let $T^+(x, n)$ be the pseudo inverse of $T(n, x) : L^2[a, b] \mapsto \mathbb{C}^n$ so that

$$T^+(x, n) = T(x, n) B^{-1}(n, n); \quad (7)$$

thus $P_n : L^2[a, b] \mapsto L^2[a, b]$ defined by the formula

$$P_n(x, y) = T^+(x, n) T(n, y) \quad (8)$$

is the orthogonal projector onto $T(n, x)$

1.2 A n -term quadrature for inner products

For a positive u , let $Q(n, x)$ denote n orthogonal basis functions for $T(n, x)$.

Definition 1.1 *A n -term quadrature $\{x_j, w_j\}$ is one with distinct x_j in $[a, b]$ and nonzero w_j , $j = 1:n$.*

Theorem 1.2 (DUALITY OF ROW AND COLUMN ORTHOGONALITIES) *Let the weight u of (5) be positive. There is a n -term quadrature $\{x_j, w_j\}$ to integrate all inner products in $T(n, x)$ if and only if the n columns of the n -by- n matrix $Q(n, \{x_j\})$ are orthogonal.*

Proof Obviously, the n -term quadrature $\{x_j, w_j\}$, if exists, integrates the Gramian $Q(n, x) \cdot Q(x, n) = I$ with positive weights w_j , namely

$$I = Q(n, \{x_j\}) \mathbf{diag}\{w_j\} Q(\{x_j\}, n) \quad (9)$$

so the n -by- n matrix $Q(n, \{x_j\}) \mathbf{diag}\{\sqrt{w_j}\}$ is unitary and thus the columns of $Q(n, \{x_j\})$ are orthogonal.

Now assume that the columns of $Q(n, \{x_j\})$ are orthogonal. Let the norm of the j -th column be $1/\sqrt{w_j}$ so that $Q(n, \{x_j\}) \mathbf{diag}\{\sqrt{w_j}\}$ is unitary, which implies that (9) holds, namely there is a n -term quadrature $\{x_j, w_j\}$ to integrate the Gramian $Q(n, x) \cdot Q(x, n) = I$; therefore it integrates all inner products in $T(n, x)$. ■

2 Construct the inner product quadrature

It is a difficult, nonlinear problem to select n orthogonal columns out of infinite number of columns of matrix Q . The selection process can be made a lot easier if the n -term quadrature is required to do a bit more. In addition to B , if the quadrature also integrates another Gramian

$$A(n, n) = T(n, x) \cdot \mu(x) T(x, n) \quad (10)$$

where μ is a simple function, then the quadrature nodes x_j will be recorded in μ . In fact, $\mu(x_j)$ will be eigenvalues of the quotient matrix AB^{-1} . We first formulate this fact in §2.1 for polynomial $T(x, n)$. The general case is treated in §2.2.

2.1 Polynomial case

Let $T(n, x)$ be the n dimensional space Π_n for polynomials of degree less than n . Let $\mu(x) = x$ so that $A(n, n)$ is given by

$$A(n, n) = T(n, x) \cdot x T(x, n) \quad (11)$$

Theorem 2.1 *If there is a n -term quadrature $\{x_j, w_j\}$ to integrate the Gramians A and B , then the nodes x_j are eigenvalues of AB^{-1}*

$$x_j = \lambda_j(AB^{-1}), \quad j = 1:n \quad (12)$$

provided that B is invertible (when u is not positive definite).

Proof The n -term quadrature exact for B is of the form

$$B = T(n, \{x_j\}) \mathbf{diag}\{w_j\} T(\{x_j\}, n) \quad (13)$$

It follows from invertibility of B that the quadrature weights w have no vanishing entry and $T(n, \{x_j\})$ is invertible; therefore,

$$\begin{aligned} AB^{-1} &= [T(n, \{x_j\}) \mathbf{diag}\{w_j x_j\} T(\{x_j\}, n)] [T(n, \{x_j\}) \mathbf{diag}\{w_j\} T(\{x_j\}, n)]^{-1} \\ &= T(n, \{x_j\}) \mathbf{diag}\{x_j\} [T(n, \{x_j\})]^{-1} \end{aligned} \quad (14)$$

Thus, the j -th eigenvalue of AB^{-1} is x_j with the eigenvector $T(n, \{x_j\})$. ■

If the weight function u is positive, then by the proof of Theorem 1.2 the quadrature weights are

$$w_j = \frac{1}{\|Q(n, x_j)\|_2^2} \quad (15)$$

If u is not positive definite, since the quadrature is exact for the first column of B , w_j will be determined by solution of the n linear equations for w

$$T(n, \{x_j\}) \mathbf{diag}\{w_j\} T(\{x_j\}, 1) = T(n, x) \cdot T(x, 1) \quad (16)$$

where $T(\{x_j\}, 1)$ is the first column of $T(\{x_j\}, n)$, and $T(x, 1) = T_1(x)$ is the first column of $T(x, n)$.

Theorem 2.2 *Let the weight function u be positive definite, and let v_j denote the j -th eigenvector of a matrix. There is a n -term quadrature $\{x_j, w_j\}$ to integrate the Gramian matrices A and B if and only if*

$$\lambda_j(AB^{-1}) = x_j, \quad j = 1:n \quad (17)$$

$$v_j(AB^{-1}) = T(n, x_j), \quad j = 1:n \quad (18)$$

Proof Only need to consider orthonormal basis $T(n, x)$ for which $AB^{-1} = A$ is Hermitian with orthogonal eigenvectors. Hence the proofs of Theorems 2.1 and 1.2 can be adopted to establish necessity and sufficiency of (17), (18). ■

Obviously, the n -term quadrature $\{x_j, w_j\}$ integrating the two Gramians integrates all polynomials of degree less than $2n$. Thus, Type-1 and Type-2 quadratures are the same for the polynomial case.

2.2 Arbitrary functions

In this section we will characterize and construct an inner product quadrature for a set of arbitrary functions $T(n, x)$.

Theorem 2.3 *Let B be invertible, and let λ_j, v_j denote the j -th eigenvalue and vector of a matrix. If there is a n -term quadrature $\{x_j, w_j\}$ to integrate the Gramians A of (10) and B , then*

$$\lambda_j(AB^{-1}) = \mu(x_j), \quad j = 1:n \quad (19)$$

$$v_j(AB^{-1}) = T(n, x_j), \quad j = 1:n \quad (20)$$

The proof is identical to that of Theorem 2.1.

Definition 2.4 *A function μ is said to be a minimal function of $T(n, x)$ if*

$$r(T, \mu) =: \mathbf{rank}\{[(I - P_n)\mu(x)T(x, n)]\} = 1 \quad (21)$$

In other words, the n functions $\mu(x)T(x, n)$ don't entirely lie in the span of $T(x, n)$, but the part of $\mu(x)T(x, n)$ that is outside of $T(x, n)$ is required to be minimal - the residual dimension $r(T, \mu)$ is 1. For example, $\mu = \exp(ix)$ is a minimal function for the subspace

$$E_m = \mathbf{span}[\exp(ikx), \quad k = -m : m], \quad m > 0, \quad x \in [-\pi, \pi] \quad (22)$$

More general definition for minimal function will be given in §3.2. Modifications are also necessary for higher dimensions.

Theorem 2.5 *Let the weight function u be positive definite, and let v_j denote the j -th eigenvector of a matrix. The three conditions are equivalent*

(i) *There is a n -term quadrature $\{x_j, w_j\}$ to integrate A and B*

(ii) *The quotient matrix AB^{-1} is diagonalizable with*

$$\lambda_j(AB^{-1}) = \mu(x_j), \quad j = 1:n \quad (23)$$

$$v_j(AB^{-1}) = T(n, x_j), \quad j = 1:n \quad (24)$$

(iii) *There exist such $\{x_j\}$ that for every $p_n \in \mathbf{span}[(I - P_n)\mu(x)T(n, x)]$*

$$p_n(x_j) = 0, \quad j = 1:n \quad (25)$$

and that the n -by- n matrix $T(n, \{x_j\})$ is invertible.

Proof The proof of equivalency of (i) and (ii) is similar to that of Theorem 2.2. Now we establish equivalency of (ii) and (iii). By (ii), and by (7) and (8),

$$\begin{aligned}
\mu(x_j)T(n, x_j) &= AB^{-1}T(n, x_j), \quad j = 1:n \\
&= T(n, x) \cdot \mu(x)T^+(x, n)T(n, x_j) \\
&= [T(n, x)\mu(x)] \cdot P_n(x, x_j) \\
&= \{P_n[T(n, x)\mu(x)]\}_{x=x_j} \\
&= \{(I - I + P_n)[T(n, x)\mu(x)]\}_{x=x_j} \\
&= T(n, x_j)\mu(x_j) - \{(I - P_n)[T(n, x)\mu(x)]\}_{x=x_j}
\end{aligned} \tag{26}$$

which holds if and only if

$$\{(I - P_n)[\mu(x)T(n, x)]\}(x_j) = 0, \quad j = 1:n, \tag{27}$$

namely (25) holds, and the n -by- n matrix $T(n, \{x_j\})$ is invertible. ■

Theorem 2.5 does not require that μ is minimal, but if it is not then all $p_n \in \mathbf{span}[(I - P_n)\mu(x)T(n, x)]$ must share n common roots at the quadrature nodes x_j . In other words, it is unlikely for a n -term quadrature to integrate both B and A exactly if μ is not minimal.

If $T(n, x) = \Pi_n$, polynomials of degree less than n , then $\mu(x) = \alpha x + \beta$, $\alpha \neq 0$ is a minimal function whereas x^2 is not. With a minimal μ , p_n of (25) is the orthogonal polynomial of degree n , provided that the weight u is positive definite. The condition (25) is well known as a part of the Gauss formula.

However, when the functions $T(n, x)$ are not polynomials, the n -term quadrature formula may not be a Gaussian quadrature in the classical sense. In general, to integrate the inner products in A and B is not the same as to integrate some $2n$ functions. Conversely, given a set of $2n$ functions to integrate by a Gaussian quadrature, additional work is required to reformulate this Type-1 quadrature as a Type-2, inner product quadrature. This issue will be addressed in the next section.

3 Product law and minimal functions

In this section we will establish framework for converting the Type-1 quadrature to Type-2, inner product quadrature. While an inner product quadrature is natural in its own right and immediately useful in many applications, other applications require Type-1 quadratures. For many familiar and widely used families of functions the two quadrature problems turn out to be equivalent or nearly so. We introduce the notion of factor space in §3.1 and minimal function in §3.2 to connect the two types of quadratures.

3.1 Factor spaces

In this section we introduce the product law and factor space for a given set of $2n$ functions, so as to convert a Type-1 quadrature for the $2n$ functions to a Type-2 for the Gramian matrix of the factor space.

Let the rows of $V(2n, x) : L^2[a, b] \mapsto \mathbb{C}^{2n}$ consist of a set of $2n$ linearly independent functions, which span a linear subspace of $L^2[a, b]$ denoted also by $V(2n, x)$.

Definition 3.1 *The linear subspace $V(2n, x)$ is said to have a factor space $T(n, x)$ with a multiplier μ if*

$$\mathbf{span}\{T_i(x)\bar{T}_j(x), T_i(x)\mu(x)\bar{T}_j(x), 1 \leq i, j \leq n\} = V(2n, x) \quad (28)$$

As an example, the linear space Π_{2n} for polynomials of degree less than $2n$ has a factor space Π_n with $\mu(x) = x$ as the multiplier. Likewise, let

$$G_m = \mathbf{span}[1, \sin(jx), \cos(jx), j = 1:m-1], \quad m > 1 \quad (29)$$

Then G_m is a factor space of G_{2m} with $\mu(x) = \cos(x)$, whereas E_m of (22) is a factor space of E_{2m} with $\mu = 1$.

Obviously, a quadrature integrating the inner products in the factor space will also integrate the functions in $V(2n, x)$. In this respect, the notion of a factor space can be relaxed in two directions (i) Let the span in (28) include, rather than equal to, $V(2n, x)$ (ii) Let the span in (28) approximate $V(2n, x)$ to a given precision.

Definition 3.2 *The linear subspace $V(2n, x)$ is said to obey the product law if there exist n functions $T(n, x)$ such that $V(2n, x)$ is a subspace of the product space*

$$\Pi(T) = \mathbf{span}\{T_i(x)\bar{T}_j(x), 1 \leq i, j \leq n\} \quad (30)$$

A linear subspace $V(2n, x)$ is said to obey the product law to precision $\epsilon > 0$ if for any $f \in V(2n, x)$ the distance between f and $\Pi(T)$ is ϵ .

As an example, by Neumann's addition formula 9.1.78 of [1],

$$J_m(x) = \sum_{k=0}^m J_k(x/2)J_{m-k}(x/2) + 2 \sum_{k=1}^{\infty} (-1)^k J_k(x/2)J_{m+k}(x/2) \quad (31)$$

For $x \in [0, b]$, and for a prescribed precision $\epsilon > 0$, there exists $\delta > 0$ so that

$$|J_s(x/2)| < \epsilon, \quad s > b + \delta \quad (32)$$

Thus, to precision $O(\epsilon)$, only finite number of terms in (31) remain: $J_s(x/2)$ for $0 \leq s \leq b + \delta$. Consequently, the space

$$\mathcal{V} = \mathbf{span}\{J_m(x), 0 \leq m \leq 2(b + \delta)\} \quad (33)$$

obeys the product law to precision $O(\epsilon)$, and a quadrature integrating the inner products in

$$\mathcal{T} = \mathbf{span}\{J_s(x/2), 0 \leq s \leq b + \delta\} \quad (34)$$

exactly or to precision $O(\epsilon)$ will also integrate functions in \mathcal{V} to precision $O(\epsilon)$.

Factor space and product law can also be extended to a family of infinite number of functions, denoted by $G(k, x)$, $x \in [a, b]$, with $k \in [\alpha, \beta]$ the family parameter.

Definition 3.3 *The family of functions $G(k, x)$ obeys the product law if there exist two families of functions $T(k, x)$, $S(\kappa, x)$, $x \in [a, b]$, $k \in [\alpha_1, \beta_1]$, $\kappa \in [\alpha_2, \beta_2]$ such that $G(k, x)$ is a subset of the product space*

$$\Pi(S, T) = \mathbf{span}\{T(k, x)S(\kappa, x), k \in [\alpha_1, \beta_1], \kappa \in [\alpha_2, \beta_2]\} \quad (35)$$

Moreover, $G(k, x)$ is said to have factor spaces $T(k, x)$ and $S(k, x)$ if

$$\mathbf{span}\{G(k, x), \alpha \leq k \leq \beta\} = \Pi(S, T) \quad (36)$$

Finally, $G(k, x)$ is said to have a factor space $T(k, x)$ if it has the factor spaces $T(k, x)$ and $S(k, x)$ with $S(k, x) = \bar{T}(k, x)$.

Accordingly, the n -by- n Gramians B of (6) and A of (10) can be extended to operator case.

Definition 3.4 *Given a function $\mu(x)$, the linear operators defined by*

$$A(k, k') = T(k, x) \cdot \mu(x) S(x, k') \quad (37)$$

$$B(k, k') = T(k, x) \cdot S(x, k') \quad (38)$$

are referred to as the Gramians associated with the factor spaces $T(k, x)$ and $S(k, x)$.

Theorem 3.5 *Let the m -by- n matrices*

$$A(m, n) = T(m, x) \cdot \mu(x) S(x, n) \quad (39)$$

$$B(m, n) = T(m, x) \cdot S(x, n) \quad (40)$$

be the Gramians associated with the m -by- $[a, b]$ matrix $T(m, x)$ and the n -by- $[a, b]$ matrix $S(n, x)$ and a scalar function μ . Let the rank of B be r . If there is a r -term quadrature

$\{x_j, w_j \mid j = 1:r\}$ precise for A and B , then the m -by- m matrix AB^+ has r eigenvalues and corresponding eigenvectors of the form

$$\lambda_j(AB^+) = \mu(x_j), \quad j = 1:r \quad (41)$$

$$v_j(AB^+) = T(m, x_j), \quad j = 1:r \quad (42)$$

The remaining $m - r$ eigenvalues are zero.

Proof The proof is similar to that of Theorem 2.1. Since B is of rank r , the existence of the r -term quadrature, exact for B , implies that the quadrature weights w have no vanishing entry and the m -by- r matrix $T_r = T(m, \{x_j\})$ and the r -by- n matrix $S_r = S(\{x_j\}, n)$ are both full rank; therefore,

$$B^+ = [T_r \mathbf{diag}\{w_j\} S_r]^+ = S_r^+ \mathbf{diag}\{w_j\}^{-1} T_r^+ \quad (43)$$

Using $S_r S_r^+ = I$ we have

$$\begin{aligned} AB^+ &= T_r \{\mu(x_j)\} \mathbf{diag}\{w_j\} S_r S_r^+ \mathbf{diag}\{w_j\}^{-1} T_r^+ \\ &= T_r \{\mu(x_j)\} T_r^+ \end{aligned} \quad (44)$$

It follows immediately that the m -by- m square matrix AB^+ , being of rank r or less, will have $m - r$ zero eigenvalues, and owing to $T_r^+ T_r = I$ the r remaining eigenvalues and vectors are given by (41), (42). \blacksquare

Theorem 2.1 is a special case of Theorem 2.3 which is a special case of Theorem 3.5. For quadrature design, we are only interested in eigenvectors, if exist, of the form $T(m, x_j)$.

Definition 3.6 The eigenvectors of AB^+ of the form $T(m, x_j)$ are referred to as the position eigenvectors.

The existence of the position eigenvectors is necessary for that of a Gaussian quadrature. The next theorem, straightforward to verify, says that the eigenvalues for the quotient matrix is invariant under the change of bases by (45), (46).

Theorem 3.7 Let the square matrices $t(m, m)$ and $s(n, n)$ be invertible. Let the change of bases, from $T(m, x)$ to $\tilde{T}(m, x)$, and from $S(n, x)$ to $\tilde{S}(n, x)$, be defined by

$$\tilde{T}(m, x) = t(m, m) T(m, x) \quad (45)$$

$$\tilde{S}(n, x) = s(n, n) S(n, x) \quad (46)$$

Then the two quotient matrices AB^+ associated with the old and new bases are similar, with $t(m, m)$ as the similarity transform.

3.2 Minimal functions

Minimal function was defined in §2.2 for a set of n functions $T(n, x)$. In this section, we will introduce minimal function for a family of infinite number of functions $G(k, x)$.

Definition 3.8 (INFORMAL) *A method to grow a family of functions G is to multiply the existing family members by a function μ , which may not be in the family. The resulting functions are linearly combined with those in the family to generate a new function. The function μ , with proper normalization, is the minimal function.*

Typical 3-term recursions use this scheme to generate a class of functions. For example, the Bessel functions require $\mu(x) = 1/x$ as the multiplier to push the family one step forward, or backward.

For a precise definition of minimal function, let the new function $G(\beta + h, x)$ be generated by linear combination of $\mu(x)G(k, x)$ and $G(k, x)$ over $k \in [\alpha, \beta]$. We scale μ such that it appears in the linear combination as follows

$$G(\beta + h, x) = hG(\beta, x)\mu(x) + G(\beta, x) + \text{tail} \quad (47)$$

The tail vanishes as $h \rightarrow 0$, provided that μ is the log derivative of G with respect to k .

Definition 3.9 *Let $G(k, x)$ be differentiable with respect to k in $[\alpha, \beta]$ for almost every $x \in [a, b]$. The function*

$$\mu(x, k)|_{k=\beta} = \left\{ \frac{\partial}{\partial k} \log G(k, x) \right\}_{k=\beta} \quad (48)$$

is referred to as a specific minimal function of $G(k, x)$ at $k = \beta$. If $\mu(x, k)$ is independent of k or if the dependence is separable

$$\mu(x, k) = p(k)q(x) \quad \text{so that} \quad \partial_k G(k, x) = p(k) G(k, x) q(x) \quad (49)$$

then it is referred to as the (general) minimal function of $G(k, x)$.

By (48), the minimal functions for the power functions (2) and exponentials (3) are $\log(x)$ and x . By μ 's dependence on k , we divide G into three varieties

(V.1) It is independent of k .

(V.2) The dependence is separable.

(V.3) The dependence is not separable.

There are two cases for constructing a quadrature, whether Type-1 or 2

(C.1) Design a quadrature with a given weight u .

(C.2) Design a quadrature without u given explicitly.

(C.1) is typical of quadrature design for numerical integration; the weight u is given explicitly. (C.2) arises from certain applications such as inverse problems or signal processing where the measurement or signal is the exact integrals

$$s(k) = \int_a^b G(k, x)u(x)dx, \quad k \in [\alpha, \beta] \quad (50)$$

with an underlying, fixed, but unknown u .

For (C.2), the only data available for Type-1 quadrature design is $s(k)$. When reformulated as a Type-2 quadrature problem, (V.1) and (V.2), not (V.3), will be useful in constructing the Gramians A and B out of the data $s(k)$. The procedures for constructing the Gramians by (V.1) and (V.2) are so similar that in the sequel we will only consider (V.1), namely (V.2) with $p(k) \equiv 1$.

For (C.1), the weight function u is given and the Gramians can be constructed directly by their definitions (37) and (38) for a Type-2 quadrature, or for a Type-1 quadrature provided that G has factor spaces $T(k, x)$ and $S(k, x)$. (V.3) will be useful for (C.1).

A specific minimal function exists for an arbitrary system of functions $G(k, x)$. In contrast, only certain function classes have (general) minimal functions. The next theorem is a direct consequence of Definition 3.9.

Theorem 3.10 *$G(k, x)$ has a minimal function if and only if*

$$G(k, x) = \exp(p(k)q(x))r(x) \quad (51)$$

Moreover, if $G(k, x)$ has a minimal function then it has a factor space

$$T(k, x) = [G(k, x)]^{1/2} = \exp(p(k)q(x)/2)\sqrt{r(x)} \quad (52)$$

For example, the family $x^k = \exp(k \log(x))$ is of this exponential type. The family $k^x = \exp(\log(k)x)$ is also of this type.

When k takes only on discrete values, say integers, the differential form (48) for μ can be replaced by a finite difference for certain classes of functions, among them are polynomials and modified Bessel functions:

$$\mu(x) = \frac{x^{n+1} - x^n}{1 \cdot x^n} = x - 1 \quad (53)$$

$$\mu(x) = \frac{I_{n+1}(x) - I_{n-1}(x)}{2 \cdot I_n(x)} = -n/x \quad (54)$$

where $x - 1$ can be normalized to x , and the separable $\mu(x, n) = -n/x$ to $1/x$.

For certain applications $k \in [\alpha, \beta]$ is restricted on a uniform grid with step size h , so that only a finite number of the family members $G(\alpha + jh, x)$, $j = 0 : n$, $nh = (\beta - \alpha)$, are to be integrated. For example,

$$\mu(x) = x^h, \quad \text{for power functions} \quad (55)$$

$$\mu(x) = e^{ihx}, \quad \text{for exponentials} \quad (56)$$

$$\mu(x) = \cos(x), \quad \text{for trigonometrics} \quad (57)$$

are appropriate minimal functions.

Remark 3.11 *The minimal function introduced in Definition 3.9 is associated with differentiation with respect to k . In general, ∂_k in (49) is replaced by a map L_k which operates on $G(k, x)$ as a family of functions of k . For example, if Sturm-Liouville equation $(-L_x + k^2)u(x) = 0$ has a solution of the form $u = G(k, x) = G(kx)$, then interchanging the roles of k and x we have $L_k G(kx) = x^2 G(kx)$. In other words, the family of functions $G(k, x) = G(kx)$ has a minimal function x^2 with respect to the operator L_k .*

3.3 Fold data into Gramians - signal processing

In quadrature design for numerical integration, the weight function u is usually prescribed. For other applications, such as optimal design or inverse problems, u is either a variable or not given explicitly.

When u is not given and the exact integrals $s(k)$ of (50) is the only available data, the first step in quadrature design for $G(k, x)$ is to process the signal s to construct the Gramians A and B .

In this section, we will describe the signal processing operations for converting Type-1 quadrature for G to Type-2 for the Gramians. This signal processing is not required to construct the Gramians if u is available.

Let $G(k, x)$ have a factor space $T(k, x)$, $k \in [\alpha_1, \beta_1]$ and a minimal function μ so that

$$\text{span}\{G(k, x), \alpha \leq k \leq \beta\} = \text{span}\{T(k, x)\bar{T}(k', x), \alpha_1 \leq k, k' \leq \beta_1\} \quad (58)$$

and

$$s'(k) = \int_a^b \mu(x) G(k, x) u(x) dx \quad (59)$$

with the latter obtained by differentiating (50). By (58), there exists linear combination coefficients $F(k, k', \kappa)$ to reproduce $T(k, x)\bar{T}(k', x)$ as a linear combination of $G(k, x)$:

$$T(k, x)\bar{T}(k', x) = \int_{\alpha}^{\beta} F(k, k', \kappa) G(\kappa, x) d\kappa \quad (60)$$

Integrating (60) with respect to x against $\mu(x)u(x)$ we rewrite the result and (59) in matrix form

$$s'(k) = G(k, x)\mu(x)u(x) \quad (61)$$

$$T(k, x) \cdot \mu(x)T(x, k') = F(k, k', \kappa)G(\kappa, x)\mu(x)u(x) = F(k, k', \kappa)s'(\kappa) \quad (62)$$

The operator $T(k, x) \cdot \mu(x)T(x, k')$, by (37), is Gramian matrix $A(k, k')$, and (62) shows that the derivative of the signal is required to construct A , and that how the vector s' is packed into A by the folding operator F . The other Gramian matrix B is also constructed by the same folding process performed on the signal s

$$A(k, k') = F(k, k', \kappa)s'(\kappa) \quad (63)$$

$$B(k, k') = F(k, k', \kappa)s(\kappa) \quad (64)$$

As an example, let $G(k, x)$ be exponentials defined by (3), which has a factor space

$$T(k, x) = \{ \exp(ikx), \quad x \in [-\pi, \pi], \quad k \in [-\beta/2, \beta/2] \} \quad (65)$$

By (60), the folding operator is

$$F(k, k', \kappa) = \delta(k - k' - \kappa), \quad k, k' \in [-\beta/2, \beta/2], \quad \kappa \in [-\beta, \beta] \quad (66)$$

so that for a fixed κ , the kernel $F(k, k', \kappa)$ is zero everywhere except on the diagonal $k - k' = \kappa$; the Gramians A and B of (63) and (64) are Toeplitz matrices with $s'(\kappa)$ and $s(\kappa)$ on the diagonal $k - k' = \kappa$.

Folding a data vector, or signal, into a matrix or matrices and subsequently processing them is inherently a data analysis procedure. When $G(k, x)$ and its factor space $T(k, x)$ share the same minimal function μ , the Gramian matrices A and B are of the form

$$B(k, k') = T(k, x) \cdot T(x, k') \quad (67)$$

$$A(k, k') = T(k, x) \cdot \mu(x)T(x, k') \quad (68)$$

$$= [\partial_k T(k, x)] \cdot T(x, k') = \partial_k B(k, k') \quad (69)$$

Theorem 3.12 *Suppose that $G(k, x)$ and its factor space $T(k, x)$ share the same minimal function μ , and that the weight function u of (5) is nonzero almost everywhere on $[a, b]$. Then the quotient matrix $Q = AB^{-1}$ is the differential operator, with respect to k , restricted on the subspace $T(k, x)$.*

If u vanishes on a subset of $[a, b]$ of positive measure, the quotient matrix Q will still be a differential operator restricted on the range space of B , which is a subspace of $T(k, x)$.

3.4 Regularization

Once the two Gramians are constructed, there are two issues with computing the quotient matrix $Q = AB^{-1}$ (i) Inverting the compact operator B (ii) For a prescribed precision $\epsilon > 0$, replace Q by a finite, n -by- n square matrix for subsequent eigen decomposition. The two issues can be tackled together by regularization of A, B : Approximate A, B with finite rank operators A_n, B_n .

Ideally, we should find a function $s_n(k)$ to approximate the data $s(k)$ in a least squares sense to the prescribed precision which when packed by (64) gives rise to B_n of rank n . Solving such a nonlinear least squares problem is not known to be tractable in cost or convergence, so suboptimal schemes are sought instead. One of them requires SVD on B with ϵ as the cut off precision to construct a rank n best approximation to B , so that

$$B(k, k') \approx U(k, n)\Sigma(n, n)V(n, k') \quad (70)$$

$$A(k, k') \approx U(k, n)S(n, n)V(n, k') \quad (71)$$

$$Q(k, k') \approx U(k, n)S(n, n)\Sigma^{-1}(n, n)U(n, k') \quad (72)$$

namely, both B and A are projected on the n dimensional column (or range) subspace spanned by $U(k, n)$ and row (or domain) space spanned by $V(k, n)$. Note that while Σ is diagonal, S is generally not. Finally, by Theorem 2.3, a n -term quadrature of finite precision proportional to the prescribed can be attempted by solving the eigenvalue problem for the projected version of Q

$$\tilde{Q}(n, n) = S(n, n)\Sigma^{-1}(n, n) \quad (73)$$

3.5 Type-3 quadratures for integral equations

Let A, B be the m -by- n Gramian matrices of Theorem 3.5. Let the rank of B be r . A r -term Type-3 quadrature uses the nodes $\{x_j, j = 1:r\}$ and weights $W = \{w_{ij} \mid i = 1:m, j = 1:r\}$ to integrate A and B

$$A(m, n) = W(m, j)\mu(x_j)S(x_j, n) \quad (74)$$

$$B(m, n) = W(m, j)S(x_j, n) \quad (75)$$

In other words, the m functions $T(m, x)$ of (37) are regarded as the weight functions for the Type-3 quadrature.

Theorem 3.13 *If there is a r -term quadrature (74), (75), then the m -by- m matrix AB^+ has r eigenvalues and corresponding eigenvectors of the form*

$$\lambda_j(AB^+) = \mu(x_j), \quad j = 1:r \quad (76)$$

$$v_j(AB^+) \propto W(m, j), \quad j = 1:r \quad (77)$$

The remaining $m - r$ eigenvalues are zero.

The proof is nearly identical to that of Theorem 3.5, and is omitted. Let

$$v(y) = \int_a^b G(y, x)u(x)dx, \quad y \in [a, b] \quad (78)$$

be an integral equation for u on $[a, b]$. Let $\{y_i, i = 1 : m\}$ be m points in $[a, b]$. Let $T(m, x) = \{G(y_i, x), i = 1 : m\}$. Finally, let $u \in S(x, n)$, namely u is in the span of the n functions S . Then W of Theorem 3.13 is a discretization of the integral equation

$$v(y_i) \approx \sum_{j=1}^r W_{ij}u(x_j) \quad (79)$$

which is precise for $u \in S(x, n)$.

4 Examples

In this section we present several examples to illustrate our quadrature design methods. In §4.1 we construct quadratures for non-positive definite weight u . §4.2 and §4.3 construct quadratures for power and exponential functions.

4.1 Quadratures for non-positive definite weights

Gaussian quadratures may not exist for non-positive definite weights. As an example, we consider n -term Gaussian quadratures to integrate polynomials of degree less than $2n$, against the weight function

$$u(x) = \sin(3\pi x) \quad (80)$$

in $[-1, 1]$. The oddness of u and the optimality of Gaussian quadrature preclude Gaussian quadratures of odd n , otherwise $x = 0$ must be a quadrature node where u vanishes which makes the node useless. Not all even n values support a Gaussian quadrature. For the weight given by (80), there is a Gaussian quadrature for $n = 16$, and $n = 18$, but not for $n = 14$. Whenever there is a Gaussian quadrature, it can be constructed by Theorem 2.1. Figure 1 shows the locations of the quadrature nodes in $[-1, 1]$, and the quadrature weights. The weights are negative wherever u is negative.

4.2 Power functions, Hankel Gramians

To integrate the power functions

$$G(k, x) = \{ x^k, \quad x \in [0, 1], \quad k \in [\alpha, \beta] \} \quad (81)$$

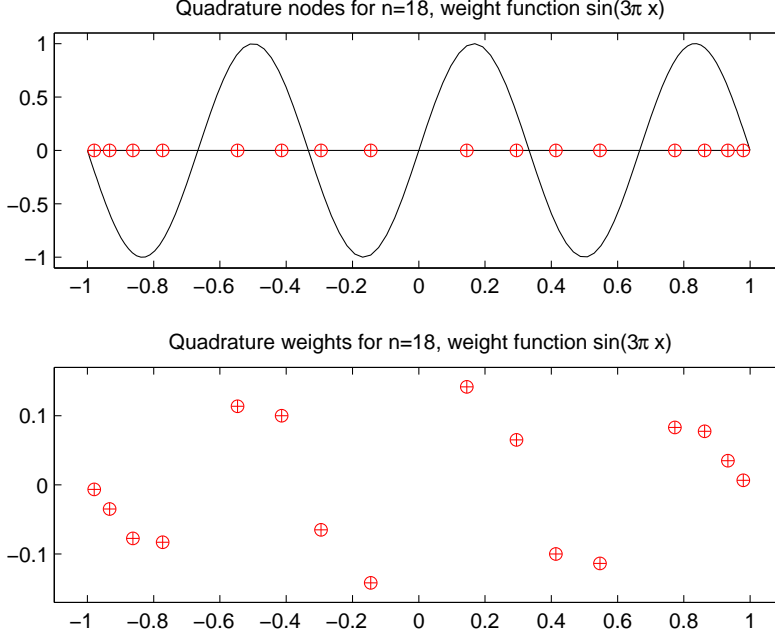


Figure 1: Quadrature nodes and weights for $u(x) = \sin(3\pi x)$

against a weight u with a n term quadrature, we follow §3.3 to construct Gramian B from the exact integrals $s(k)$, and Gramian A from $s'(k)$.

By (48), the minimal function is $\mu(x) = \log(x)$. The power functions obey the product law of Definition 3.3, with

$$T(k, x) = \{ x^k, \quad x \in [0, 1], \quad k \in [\alpha/2, \beta/2] \} \quad (82)$$

By (60), the folding kernel F , cf (66), is

$$F(k, k', \kappa) = \delta(k + k' - \kappa), \quad k, k' \in [\alpha/2, \beta/2], \quad \kappa \in [\alpha, \beta] \quad (83)$$

Therefore, the Gramians A and B are Hankel matrices with $s'(\kappa)$ and $s(\kappa)$ on their anti-diagonals $k + k' = \kappa$.

For a numerical experiment, we construct a Gaussian quadrature for $G(k, x) = x^k$, $x \in [a, b] = [0, 1]$, $k \in [\alpha, \beta] = [-1/3, 1/2]$ by constructing an inner product quadrature for the factor space $T(k, x) = k^x$, $x \in [a, b] = [-3, 3]$, $k \in [\alpha/2, \beta/2] = [-1/6, 1/4]$. Following the procedures of §3.4, a n term quadrature, though not precise to integrate all functions in $G(k, x)$, was constructed from the n -by- n Gramians A and B of (70). For a cut off precision $\epsilon = 10^{-12}$, $n = 9$. Figure 2 shows the locations of nodes in $[-3, 3]$, and the relative error of the quadrature as a function of $k \in [1/16, 4]$.

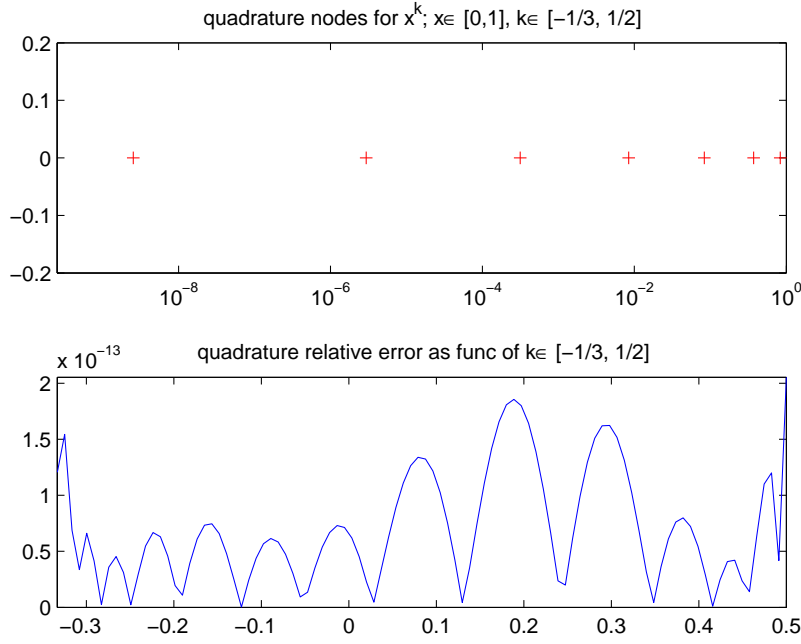


Figure 2: Quadrature nodes and relative error for $G(k, x) = x^k$

4.3 Exponentials k^x , hyperbolic Gramians

This subsection is analogous to the preceding one; therefore, we will only provide the essentials. The family of exponential functions

$$G(k, x) = \{ k^x, \quad x \in [a, b], \quad k \in [\alpha, \beta] \}, \quad \alpha > 0 \quad (84)$$

is not equivalent to $\exp(kx)$. The minimal function is dependent on k but the dependence is separable

$$\mu(x, k) = x/k := \mu(x)/k \quad (85)$$

The factor space

$$T(k, x) = \{ k^x, \quad x \in [a, b], \quad k \in [\sqrt{\alpha}, \sqrt{\beta}] \} \quad (86)$$

gives rise to the folding kernel

$$F(k, k', \kappa) = \delta(kk' - \kappa), \quad k, k' \in [\sqrt{\alpha}, \sqrt{\beta}], \quad \kappa \in [\alpha, \beta] \quad (87)$$

Therefore, the Gramians $A(k, k')$ and $B(k, k')$ are operators with $\kappa s'(\kappa)$ and $s(\kappa)$ on the hyperbolae $kk' = \kappa$. For constant weight $u = 1$,

$$s(k) = \frac{k^b - k^a}{\ln k}, \quad ks'(k) = \frac{bk^b - ak^a}{\ln k} - \frac{s(k)}{\ln k} \quad (88)$$

For a numerical experiment, we construct a Gaussian quadrature for $G(k, x) = k^x$, $x \in [a, b] = [-3, 3]$, $k \in [\alpha, \beta] = [1/16, 4]$ by constructing an inner product quadrature for the factor space $T(k, x) = k^x$, $x \in [a, b] = [-3, 3]$, $k \in [\sqrt{\alpha}, \sqrt{\beta}] = [1/4, 2]$. For a cut off precision $\epsilon = 10^{-12}$, the procedures of §3.4 gives rise to $n = 9$. Figure 3 shows the locations of nodes in $[-3, 3]$, and the relative error of the quadrature as a function of $k \in [1/16, 4]$.

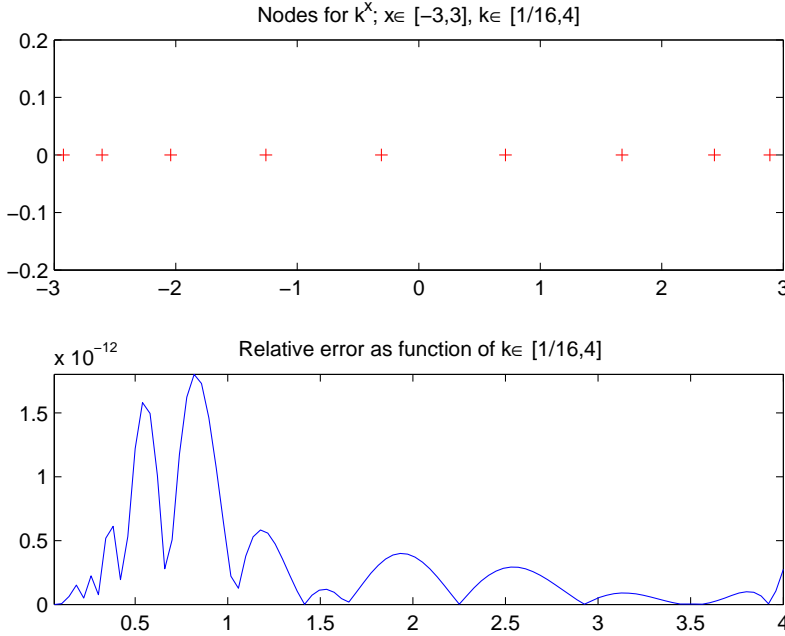


Figure 3: Quadrature nodes and relative error for $G(k, x) = k^x$

5 Generalizations and applications

The algorithms for the inner product quadrature design, presented in Theorem 2.3, 2.3, and 3.5, will also work for matrix and tensor quadrature weights. Take the two Gramians A, B of Theorem 3.5 for example, the product space $\Pi(S, T)$ of (35) may have a dimension on the order mn . A quadrature of r nodes, with $r \leq m$, will integrate these $O(mn)$ distinct functions only if the quadrature weights w has off diagonal entries. It may be a banded matrix, or a dense matrix with a predetermined diagonals, but as long as the r -by- r matrix w is invertible, Theorem 3.5 still holds, for its proof is equally valid as the diagonal matrix w is replace by an invertible one.

Tensor “weights” refer to one or two r -by- r matrix w which will entrywise multiply the integrand T_r from the right, or S_r from the left, or both, as opposed to standard matrix-matrix multiplication. The proof of Theorem 3.5 holds, as T_r and S_r will still be full rank r after the entrywise multiplication, otherwise the rank of B will be less than r .

Matrix and tensor quadrature weights are related to certain sensing and inverse scattering applications; see §5.1 for more details.

The 1-D results presented in this paper makes a step toward a systematic method to design Gaussian quadratures for an arbitrary system of functions in one and higher dimensions; see §5.2 and 5.3 for 2-D extensions.

5.1 Separation principle of imaging

The mathematical models for imaging, with the notable exceptions of MRI and X-ray CAT scan due to absence of wave scattering as their probing mechanisms, are inconsistent in that their formulation is based on reflectivity or scattering coefficient of targets as a function of position. But in many applications, these functions are not nearly single valued. Amplitude of backward, monostatic reflected wave from a small target depends on direction unless the target is a ball, for example, with uniform reflection coefficient on the sphere.

There is a remarkable property of Gaussian quadrature design - the nodes can be determined *first* and *independently* of the weights. This is also valid for a “quadrature” with inconsistent “quadrature weights”, namely with tensor weights. For imaging or inverse scattering with waves, the measurement is typically a Gramian matrix known as the scattering matrix. For some r point targets as the scatterers, there is a r -term quadrature to integrate the Gramian matrix, and the quadrature nodes fall on the locations of the point targets, provided that the size of the Gramian matrix is no less than r . Thus, the quadrature approach presents an alternative model based on the locations of targets.

If we construct a quadrature for the Gramian matrix, the locations of the targets will be determined *first* and *separately* from the target’s reflectivities, whether or not they are consistent. If consistent, and if there is no multiple scattering among them then the quadrature weights will be the reflectivities; if there is multiple scattering then the quadrature weights will be a dense matrix which together with the quadrature nodes will be sufficient to recover the consistent reflectivities via solution of a simple matrix equation. If the reflectivities are inconsistent, the quadrature weights will be tensor, and it is possible to assign an average reflectivity to each point target.

5.2 Quadratures in higher dimensions

A Gaussian quadrature in two dimensions integrating the bivariate polynomials of degree less than $2n$ in a domain D , as is well known, is a summation of $n(n+1)/2$ terms. Such a quadrature rarely exists. We will, however, provide a 2-D versions of Theorems 2.1 and 2.2 to construct the quadrature by eigen decomposition, and to illustrate what is required of quadrature design in higher dimensions. The results will also be useful in §5.3 for quadrature in two and higher dimensions constructed by a technique called deflation.

Let $T(n, x, y)$ of size $n(n+1)/2$ -by- D be the $n(n+1)/2$ basis functions for polynomials of degree less than n in the domain D . Let

$$B = T(n, x, y) \cdot T(x, y, n) \quad (89)$$

$$A_x = T(n, x, y) \cdot xT(x, y, n) \quad (90)$$

$$A_y = T(n, x, y) \cdot yT(x, y, n) \quad (91)$$

where the dot product is over domain D and with a weight function u . We have

Theorem 5.1 *If there is a $n(n+1)/2$ -term quadrature $\{(x_j, y_j); w_j\}$ to integrate the Gramian matrices B , A_x , and A_y , then*

$$\lambda_j(A_x B^{-1}) = x_j, \quad j = 1:n(n+1)/2 \quad (92)$$

$$\lambda_j(A_y B^{-1}) = y_j, \quad j = 1:n(n+1)/2 \quad (93)$$

Here the weight u is not assumed positive. This result will be useful in §5.2 for deflating the Gramians.

Theorem 5.2 *Let the weight function u be positive definite, and let v_j denote the j -th eigenvector of a matrix. The three conditions are equivalent*

(i) *There is a $n(n+1)/2$ -term quadrature $\{(x_j, y_j); w_j\}$ to integrate B , A_x , and A_y .*

(ii) *The two quotient matrices share common eigen space, and*

$$\lambda_j(A_x B^{-1}) = x_j, \quad j = 1:n(n+1)/2 \quad (94)$$

$$\lambda_j(A_y B^{-1}) = y_j, \quad j = 1:n(n+1)/2 \quad (95)$$

$$v_j(A_x B^{-1}) = v_j(A_y B^{-1}) = T(n, x_j, y_j), \quad j = 1:n(n+1)/2 \quad (96)$$

(iii) *The $n+1$ orthogonal polynomials of degree n have $n(n+1)/2$ real, pairwise distinct, common zeros $\{(x_j, y_j), j = 1:n(n+1)/2\}$.*

The proof of equivalency of (i) and (ii) is similar to that of Theorem 2.2. For (iii), see the proof of Theorem 2.5.

5.3 Deflation for 2-D quadrature design

A node of a 2-D quadrature provides 3 parameters $\{(x_j, y_j); w_j\}$. Denote by $P_n^{(2)}$ the linear space of bivariate polynomials of degree less than n . Therefore,

$$\mathbf{dim}(P_n^{(2)}) = n(n+1)/2, \quad \text{and} \quad \mathbf{dim}(P_{2n}^{(2)}) = n(2n+1) \quad (97)$$

A quadrature integrating $P_{2n}^{(2)}$ generally requires no less than a third as many nodes as the dimension, namely $n(2n+1)/3$ nodes.

A classical Gaussian quadrature for bivariate polynomials, if exists, can be constructed by Theorem 5.1, using $n(n+1)/2$ nodes to integrate $P_{2n}^{(2)}$; therefore, the quadrature problem is over-determined and rarely has a solution. The algorithm of Theorem 5.1 is rarely useful. But it can be modified and made useful by deflating the Gramians A and B iteratively.

The eigen decomposition of Theorem 5.1 can only provide $n(n+1)/2$ nodes. Additional nodes will be determined by other mechanisms. The number of these nodes is

$$dN = n(2n+1)/3 - n(n+1)/2 = n(n-1)/6 \quad (98)$$

which is about a third of $n(n+1)/2$, namely a third of what can be provided by the eigen decomposition. In 3-D, the ratio is 1; as many additional nodes are requires as those by the eigen decomposition. Deflation is a method to provide the additional nodes iteratively. The following description takes bivariate polynomials in a triangle as example to illustrate the method.

1. Suppose that a total of 40 nodes are required to integrate polynomials of degree less than $2n$ for some n . Suppose that the size of Gramians is 30, so eigen decomposition can only provide 30 nodes. Additional 10 nodes will be supplied by an iterative procedure.
2. Suppose we are given the precise locations of 10 out of the 40 nodes and the corresponding weights w_j . Each node $z_j = (x_j, y_j)$, $j = 1:10$, gives rise to a rank one matrix $T(n, z_j)w_jT(z_j, n)$; see Theorem 5.1 for notation. Deflation involves three steps (i) Remove these 10 matrices from Gramian B (ii) Remove the 10 rank one matrices $T(n, z_j)w_jx_jT(z_j, n)$ from Gramian A_x (iii) Remove the 10 rank one matrices $T(n, z_j)w_jy_jT(z_j, n)$ from Gramian A_y .
3. Theorem 5.3 below states that the eigen decomposition on the quotient matrices A_xB^{-1} and A_yB^{-1} (cf Theorem 5.1) after the deflations will provide the exact locations of the remaining 30 nodes.
4. Initialization. Choose 10 nodes and weights as initial guess. There are ways to make good initial guess located in a corner of the triangle - the domain of integration.

5. Iteration. Eigen decomposition of the deflated quotient matrices to obtain 30 nodes. Discard 20 of them by choosing only 10 out of 30 that are farthest from the 10 initial guess, and use them as the initial guess for the next iteration.
6. Convergence. The Coulomb potential $1/r$ decays over distance. Its perturbation due to that of charge location decays faster: $1/r^2$. The location errors in the 10 initial guess will have minimal influence on the farthest of the 30 nodes.

Deflation is also useful for constructing (i) Gauss-Radau type formula (with an end $x=a$ or b fixed as a quadrature node) in one and higher dimensions (ii) Gauss-Lobatto type formula (with two ends fixed as quadrature nodes) in one and higher dimensions.

Deflation can be used for constructing a Gaussian quadrature in a submain and merging it to an existing quadrature as the trapezoidal rule in another subdomainsuch - the so-called hybrid rules [3].

Theorem 5.3 *Suppose there is a $n(n+1)/2 + r$ -term quadrature $\{(x_j, y_j); w_j\}$ to integrate the Gramians B , A_x , and A_y of (89)-(91). For the first r nodes, let the deflated Gramians be defined by*

$$\dot{B} = B - \sum_{j=1}^r T(n, x_j, y_j) w_j T(x_j, y_j, n) \quad (99)$$

$$\dot{A}_x = A_x - \sum_{j=1}^r T(n, x_j, y_j) w_j x_j T(x_j, y_j, n) \quad (100)$$

$$\dot{A}_y = A_y - \sum_{j=1}^r T(n, x_j, y_j) w_j y_j T(x_j, y_j, n) \quad (101)$$

then

$$\lambda_j(\dot{A}_x \dot{B}^{-1}) = x_j, \quad j = 1 + r : n(n+1)/2 + r \quad (102)$$

$$\lambda_j(\dot{A}_y \dot{B}^{-1}) = y_j, \quad j = 1 + r : n(n+1)/2 + r \quad (103)$$

The proof is a direct consequence of Theorem 5.1 applied to the deflated weight function

$$\dot{u}(x) = u(x) - \sum_{j=1}^r w_j \delta(x - x_j, y - y_j) \quad (104)$$

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